Solution Thermodynamics of Organic Solutes in Propylene Glycol Phenyl Ether Determined by Gas-Liquid Chromatography

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The solution thermodynamics of 17 organic solutes were studied in propylene glycol phenyl ether by gas-liquid chromatography. The glycol ethers represent a unique group of solvents that can be functionalized to provide both hydrophobic and hydrophillic interaction abilities. The specific glycol ether used in this study is functionalized with a phenyl substituent, rendering it very hydrophobic in nature. Values for the infinite dilution activity coefficients (fully corrected for vapor phase nonidealitiy) of the 17 solutes were determined from the chromatographic measurements. From the measured infinite dilution activity coefficients the excess Gibbs free energies of solution were calculated. In addition, the enthalpies of solution and enthalpies of mixing for the solutes were determined from standard thermodynamic relationships. We have attempted to model the nonideality of the propylene glycol phenyl ether solutions using both UNIFAC and solute interaction parameters. The infinite dilution activity coefficient values were predicted by UNIFAC and compared to the measured chromatographic values. The excess Gibbs free energy was modeled using a linear solvation energy relationship (LSER) as a function of the solute molecular interaction parameters. Results of the comparison between UNIFAC and the LSER will be discussed.